Recent work with RAJA, and a nested loop update

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RAJA is a C++ abstraction layer that enables portability with small disruption to application programming styles

The main goal of RAJA is to balance *performance*...

- Preserve and augment abilities of C++ compilers to optimize
- Support various forms of fine-grained (on-node) parallelism and various programming model options (OpenMP, CUDA, TBB, OpenACC, ...)

... and *developer productivity*

- Maintain single-source kernels and don't bind an app to a particular PM
- Clear separation of responsibilities
 - RAJA: Execute loops, encapsulate hardware & programming model details
 - Application: Select loop iteration patterns and execution policies with RAJA API

RAJA development is currently driven by the needs of ATDM/ASC applications at LLNL and ECP collaborators





RAJA concepts help encapsulate loop execution details

C-style for-loop

```
double* x ; double* y ;
double a, tsum = 0, tmin = MYMAX;

for ( int i = begin; i < end; ++i ) {
    y[i] += a * x[i] ;
    tsum += y[i] ;
    if ( y[i] < tmin ) tmin = y[i];
}</pre>
```

RAJA decouples loop iteration and loop body

Iterations are "tasks" – aggregate, reorder, etc.

RAJA Concepts:

- Patterns: forall, forallN, reduce, scan
- Policies: sequential, simd, openmp, cuda,
- Index: iterations aggregate, reorder, tile,

RAJA-style loop

```
double* x ; double* y ;
double a ;
RAJA::SumReduction<reduce_policy, double> tsum(0);
RAJA::MinReduction<reduce_policy, double> tmin(MYMAX);

RAJA::forall< exec_policy > ( IndexSet , [=] (int i) {
    y[i] += a * x[i] ;
    tsum += y[i];
    tmin.min( y[i] );
} );
```

Execution patterns & policies (scheduling, PM choice, etc.)

IndexSets

(iteration space, ordering, etc.)

Portable Reduction types

Loop body is mostly unchanged (C++ lambda function).





Why we prefer RAJA over alternatives

- "Light touch"
 - Existing application data structures & algorithms require little change, if any
- "Low barrier to entry"
 - Parallelism can be added selectively and performance tuned incrementally
- "Application-facing design philosophy"
 - Maps naturally to apps and can be customized easy to grasp for (non-CS) application developers
- "Performance"
 - RAJA does well with "streaming" kernels that are prevalent in LLNL codes
 - Designed for coarse-grained synchronization reduces resource contention and memory synchronization overheads



RAJA developments since last year and WIP

- Cleaner organization of concepts & header files, refined APIs
- Backends for OpenMP4.x, OpenACC, TBB
- Parallel scans
- New IndexSet implementation supports arbitrary segment types
- "Multi-policy" for runtime policy selection
- Improved integration with CHAI
- RAJA Performance Suite run various experiments to compare kernels (RAJA vs. native), help guide compiler NRE work
- Expanded and refined nested loop capabilities and API



Nested loop roadblocks

- Recent work with NVidia nvcc, IBM hackathon at LLNL
 - Identified performance issues in nested-loop abstractions (RAJA::forallN)
 - Copy construction of loop body
 - Capture-by-value vs. capture-by-reference causing issues with nvcc correctness

Rework of forallN

- Current implementation of forallN relies on a "peel and bind" mechanism to generate the nested loop structure and bind the loop iterates to the lambda
 - Causes excessive copy construction seen as massive performance problem with things like CHAI, host-device lambdas, reduction object.
- Revamp of forallN replaces "peel and bind" with "peel and set" mechanism that doesn't trigger copy construction



Current Peel-and-Bind implementation of RAJA::forallN

```
For i : I
For j : J
For k : K
body(i,j,k)
```

```
auto body = [=](int i, int j, int k){ ... };
RAJA::forallN<pol>(I, J, K, body);
```

- Each loop performs two capture-by-value wrappings of the loop body
 - One peels off that loops execution policy and segment
 - The other binds that loops iterate to the body (similar to std::bind)
 - Number of copy-constructions of body O(I*J*K)

```
A = IndexConverter(body)
B = PeelOuter(A)
For i : I
    C = BindFirstArg(A, i)
    D = PeelOuter(C)

For j : J
    E = BindFirstArg(C, j)
    F = PeelOuter(E)

For k : K
    G = BindFirstArg(E, k)
    G()
```



Why was Peel-and-Bind used if it's so inefficient?!?

- It was straightforward to design
 - An initial implementation
- We just didn't know
 - Often the "body" is a lambda which only captures POD types
 - · The compiler can eliminate most of the copy constructors and inline everything
 - There is no apparent inefficiency
- So what happened?
 - Three things:
 - We used RAJA reduction objects
 - We used CHAL
 - CUDA host-device lambdas
 - These have explicit copy constructors
 - The compiler does not optimize these away
 - Performance drops through the floor

We only see performance loss when our lambdas capture complex objects





Reengineered nested loop execution invokes the loop body with a tuple of indices

```
For i : I
For j : J
For k : K
body(i,j,k)
```

```
auto body = [=](int i, int j, int k){ ... };
RAJA::forallN<pol>(I, J, K, body);
```

- Each loop assigns its iterate into a tuple
 - One wrapping of body is needed to provide invocation
 - Wrapper can be captured-by-reference at each loop nest level
 - Number of loop-body copy constructions is O(1)
 - Side Benefit: New portable metaprogramming library "camp"

```
idx = std::tuple<int, int, int>
A = InvokeWrapper(body)
For i : I
  idx.i = i

For j : J
  idx.j = j

For k : K
  idx.k = k

A(idx)
```



Conclusion

- A lot of things are going on in RAJA
 - New features
 - New backends
- Running up against performance portability issues with CUDA and OpenMP 4.5 that are forcing us to rethink certain implementation strategies
- Bug reports, feature requests, code contributions, are all welcome!
- Get RAJA on github:
 - https://github.com/LLNL/RAJA



Number of loop-body copy constructions for the Peel-and-Bind implementation

$$Copies(I_0) = 2 + ||I_0||$$

$$Copies(I_0, I_1) = 2 + 2||I_0|| + ||I_0 \times I_1||$$

$$Copies(I_0, I_1, I_2) = 2 + 2||I_0|| + 2||I_0 \times I_1|| + ||I_0 \times I_1 \times I_2||$$

Copies(
$$\{I_i\}$$
) = 2 + $\left(\sum_{i=1}^{N} 2 \prod_{j=1}^{i} ||I_j||\right) + \prod_{j=1}^{N} ||I_j||$

$$= \mathcal{O}\left(\prod_{j=1}^{N} ||I_j||\right)$$

The number of copy-ctors called is on the order of the iteration space size



